Mathematical modeling of concrete carbonation process with hysteresis effect (Analysis on non-equilibria and nonlinear phenomena : from the evolution equations point of view)

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Mathematical modeling of concrete carbonation process with hysteresis effect

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1 Introduction

From civil engineering point of view it is very important to investigate concrete carbonation process. On this subject Böhm and Muntean have already proposed a one-dimensional free boundary as a mathematical model for concrete carbonation and discussed the well-posedness of the problem, mathematically, in [16, 17]. Recently, the simplified model of the problem are studied in [4, 5, 6, 7, 8, 9, 10]. In particular, one of these results is concerned with large time behavior which guarantees that the $\sqrt{t}$-law for carbonation front is true. Here, we note that $\sqrt{t}$-law is well-known as an experimental result and means that the carbonation front behaves like $\sqrt{t}$ for sufficiently large t. In such previous results hysteresis effect are neglected, although we can find hysteresis loops in graphs of some relationships between parameters obtained by experiments. The aims of this paper are to show a mathematical modeling process for concrete carbonation process on a 3-dimensional domains with consideration of hysteresis effects and to review recent results on this model. Our modeling is due to Maekawa-Ishida-Kishi [15], Maekawa-Chaube-Kishi [14] and Muntean [16].

The outline of carbonation process can be described as follows: $CO_2(g)$ from the atmosphere enters the porous structure of concrete-based materials via the air parts of the pore where it quickly dissolves in pore water, that is

$$CO_2(g) \leftrightarrow CO_2(aq). \tag{1.1}$$

In the pore water, $CO_2(aq)$ reacts fast with available alkaline species (in particular with $Ca(OH)_2(aq)$), i.e.

$$CO_2(aq) + Ca(OH)_2(aq) \rightarrow H_2O + CaCO_3(aq). \tag{1.2}$$

From the reaction formula (1.2) we conclude that we need differential equations describing the conservation laws for moisture and carbon dioxide in order to establish a mathematical model for concrete carbonation. Then we shall discuss the conservation laws for moisture in section 2 and carbon dioxide in section 3.

Throughout this paper we use the following notations: t is time, u, v, w and y are concentrations of CO_2 in water and in air, $Ca(OH)_2$ and $CaCO_3$ in water, respectively, p is the pore pressure, ρ_l is the density of liquid, R is the gas constant, θ is the temperature

(given constant), M_l is the molecular mass of liquid, and h is the relative humidity. In [15, p. 121] they assume that

$$p = \frac{\rho_l R\theta}{M_l} \log h.$$

Then we can put $p = C_l \log h$ in this paper, where $C_l = \frac{\rho_l R\theta}{M_l}$.

2 Conservation law for moisture

In this section we formulate a moisture transport model under consideration the multi-phase dynamics of liquid and gas phases.

First, the conservation law for moisture is given as follows (see [15, p. 120] and [14, (4.2) in Chapter 4]):

$$\frac{\partial}{\partial t}(\rho_l \phi S_l) + \operatorname{div} J_w = Q_{hyd}, \tag{2.1}$$

where ϕ, S_l, J_w and Q_{hyd} are functions describing the porosity, the degree of saturation, the flux of moisture and water consumption due to hydration, respectively. Moreover, it is supposed that $\phi = \phi(z)$, where z the ration of amount of consumed $Ca(OH)_2$ for total amount of $Ca(OH)_2$ (see [15, (23)]), and ϕ is a continuous function on $\mathbf{R}$ satisfying

$$\phi \geq \phi_0 > 0 \text{ and } \phi' \geq 0 \quad \text{on } \mathbf{R},$$

where ϕ_0 is a positive constant. The typical example of ϕ is given as Figure 1.

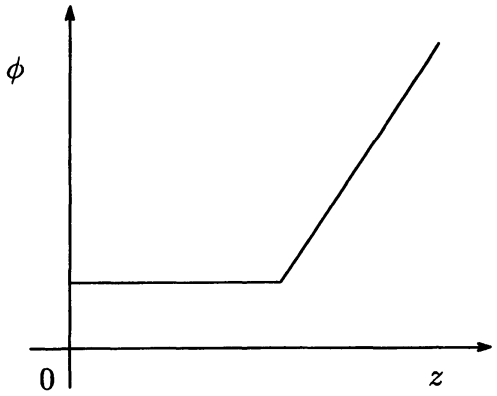

Figure 1.

Since we consider the dynamics of liquid and gas phases, the flux of moisture is described with the sum of he fluxes of moisture due to and liquid q_l and vapour q_v phases, that is,

$$J_w = q_l + q_v.$$

On account of the statement in [15, p.120] and [14, (4.53)] we assume that

$$q_l = -K_l \nabla p, \quad K_l = \frac{\rho_l \phi^2}{50\eta} \left(\int_0^{r_c} r dV \right)^2,$$

where K_l is the liquid conductivity, η is the viscosity of fluid under non-ideal conditions, r is the pore radius, r_c is the pore radius in which the equilibrated interface of liquid and

vapor is created and V is the normalized pore volume. Here, η is given by $\eta = a(1+H_d^2)$, where a is a positive constant and H_d is determined by a hysteresis operator $\mathcal{H}_0$ with the input function h, that is, $H_d = \mathcal{H}_0(h)$. Then we may assume that for some hysteresis operator $\mathcal{H}$

$$\eta = \mathcal{H}(h), \quad 0 < a \leq \mathcal{H}(h) \leq a(1+b),$$

where b is a positive constant.

Next, from [15, p.121] and [14, p.46] we have $r_c = -\frac{2\gamma}{p}$ and $V = 1-\exp(-Br)$, where γ and B are given positive constants. Accordingly, we obtain

$$\begin{aligned}\int_0^{r_c} r dV &= \int_0^{r_c} rV'(r)dr \\ &= \int_0^{r_c} (Br)\exp(-Br)dr \\ &= \frac{1}{B}(\frac{2B\gamma}{p}\exp(\frac{2B\gamma}{p}) - \exp(\frac{2B\gamma}{p}+1)).\end{aligned}$$

By using $p = C_l \log h$, we see that

$$\int_0^{r_c} r dV = \frac{1}{B}(\frac{2B\gamma}{C_l \log h}\exp(\frac{2B\gamma}{C_l \log h}) - \exp(\frac{2B\gamma}{C_l \log h})+1)$$

so that

$$K_l = \frac{\rho_l \phi^2}{50B^2\mathcal{H}(h)}\left(\frac{2B\gamma}{C_l \log h}\exp(\frac{2B\gamma}{C_l \log h}) - \exp(\frac{2B\gamma}{C_l \log h})+1\right)^2.$$

On the flux of moisture due to vapor phase movement it holds that

$$q_v = -K_v \nabla p,$$

where K_v is the vapor conductivity. In [15] they suppose that

$$K_v = \hat{K}_v \phi(1-S)h,$$

where $\hat{K}_v$ is a positive constant. From the above argument we observe that

$$J_w = -(K_l + K_v)C_l \frac{\nabla h}{h}. \tag{2.2}$$

From now on in order to be able to deal with (2.2) by the system of partial differential equations we give some estimates for $\frac{K_l}{h}$ and $\frac{K_v}{h}$. We may assume that $0 \leq h \leq 1$, physically. By putting

$$\bar{K}_l(h) = \left(\frac{C_B}{\log h}\exp(\frac{C_B}{\log h}) - \exp(\frac{C_B}{\log h})+1\right)^2,$$

where $C_B = \frac{2B\gamma}{C_l}$, and elementary calculations we can show

$$\lim_{h \downarrow 0}\frac{\bar{K}_l(h)}{h} = +\infty, \quad \lim_{h \uparrow 0}\frac{\bar{K}_l(h)}{h} = 1.$$

and there exists a positive constant $\bar{\kappa}$ such that

$$\frac{\bar{K}_l(h)}{h} \geq \hat{\kappa} \quad \text{for } 0 < h \leq 1.$$

Due to [16, (2.61)] the right hand side of (2.1) is supposed that

$$Q_{hyd} = \phi S([u]^+)^{q_1}([w]^+)^{q_2},$$

where q_1 and q_2 are positive constants with $q_1, q_2 \geq 1$. We note that S is determined by the hysteresis operator $\mathcal{S}$ with input function h (see [14, Figure 4.10, p.79]). Also, we may assume that $0 \leq \mathcal{S}(h) \leq 1$.

Thus we have the following partial differential equation as the description of the mass conservation law for moisture:

$$\rho_l \frac{\partial}{\partial t}(\phi S) - \operatorname{div}\left(\left(\frac{\hat{K}_l(h)\phi(z)^2}{\mathcal{H}(h)} + \hat{K}_V C_l \phi(z)(1-S)\right)\nabla h\right) = \phi(z) S([u]^+)^{q_1}([w]^+)^{q_2}, \quad (2.3)$$

where $\hat{K}_l(\cdot)$ is a continuous function on the interval $(0, 1]$ satisfying $\lim_{h \downarrow 0} \hat{K}_l(h) = +\infty$ and $\hat{K}_l \geq \hat{\kappa} > 0$ on $(0, 1]$ for a positive constant $\hat{\kappa}$.

3 Conservation law for carbon dioxide

The aim of this section is to provide a partial differential equation for a mathematical description of the mass conservation law for carbon dioxide. A part of the following discussion was already shown in [13].

First, the conservation law and Fick's first law lead to

$$\frac{\partial}{\partial t}(\phi((1-S)v + Su)) + \operatorname{div} J_c = Q_g, \quad J_c = -(D_{gc}\nabla v + D_{dc}\nabla u),$$

where J_c is the flux of gaseous and dissolved carbon dioxide, D_{gc} and D_{dc} are diffusion coefficients of gaseous and dissolved CO_2 in the porous media and Q_g is representing the consumption rate of carbon dioxide. In [16, 17] for the reaction (1.1) it is supposed that Henry's law holds only in stable state. Now, we assume that Henry's law is always valid. This assumption implies that $p_c = H_c u$, where p_c is the pressure of carbon dioxide in air and H_c is Henry's constant for carbon dioxide. Also, by using ideal gas law we can obtain

$$v = \frac{H_c M_c}{RT} u,$$

where M_c is the molecular mass of carbon dioxide. Thus we can rewrite the flux of gaseous and dissolved carbon dioxide as follows:

$$J_c = -(D_{gc}\frac{H_c M_c}{RT} + D_{dc})\nabla u.$$

Due to [15, p. 120] D_{gc} and D_{dc} have the following forms:

$$D_{gc} = K_g \phi(1-S), \quad D_{dc} = K_d \phi S,$$

where K_g and K_d are given positive constants. Also, from the chemical reaction theory the consumption rate of carbon dioxide Q_g satisfies

$$Q_g = \frac{\partial[\mathrm{CaCO_3}]}{\partial t} = \kappa[\mathrm{Ca^{2+}}][\mathrm{CO_3^{2-}}],$$

where κ is the reaction rate coefficient of carbonation and $[a]$ indicates the concentration of the element a. Here, by observing (1.2) we obtain that the sum of mol concentrations of $\mathrm{CaCO_3}$ and $\mathrm{Ca(OH_2)}$ is conserved so that

$$\frac{1}{M_1}[\mathrm{Ca(OH)_2}] + \frac{1}{M_2}[\mathrm{CaCO_3}] = \text{ constant},$$

where M_1 and M_2 are the molecular masses of $\mathrm{Ca(OH)_2}$ and $\mathrm{CaCO_3}$. By regarding that $\frac{w}{M_2} = \frac{[\mathrm{Ca^{2+}}]}{M_3}$ and $\frac{u}{M_4} = \frac{[\mathrm{CO_3^{2-}}]}{M_5}$ where M_3, M_4 and M_5 are the molecular masses of $\mathrm{Ca^{2+}}$, $\mathrm{CO_2}$ and $\mathrm{CO_3^{2-}}$, we see that

$$-\mu_1 \frac{\partial y}{\partial t} = \frac{\partial w}{\partial t} = -\kappa_1 uw,$$

where μ and κ_1 are positive constants. By solving this ordinary differential equation we obtain

$$w(t) = w(0)\exp(-\kappa_* \int_0^t u(\tau)d\tau).$$

where κ_* is a positive constant.

As mentioned before, z is defined by

$$z(t) = \frac{w(0) - w(t)}{w(0)} \quad \text{so that} \quad z(t) = 1 - \exp(-\kappa_* \int_0^t u(\tau)d\tau).$$

Hence, we have the following partial differential equation:

$$\frac{\partial}{\partial t}(\phi(\rho_0(1-S)+S)u) - \operatorname{div}(\phi(\rho_1 K_g(1-S)+K_d S)(\nabla u)) = -\kappa_1 uw, \tag{3.1}$$

with

$$w(t) = w(0)\exp(-\kappa_* \int_0^t u(\tau)d\tau), \phi = \phi(1 - \exp(-\kappa_* \int_0^t u(\tau)d\tau)).$$

4 Review of mathematical results

As we discussed in sections 2 and 3, we obtain the system {(2.3), (3.1)} as a mathematical model for concrete carbonation. Since both equations include hysteresis operators, it is not easy to deal with the system, directly, so that we studied the simplified equations of (2.3) and (3.1) as a first step of this research. In this section we show our previous results concerned with these equations.

First, we consider the equation corresponding to the conservation law of moisture. In [1] we treated the simplified equation of (2.3) as follows:

$$\rho\frac{\partial h}{\partial t} - \operatorname{div}(g(h)\nabla h) = wf, w = \mathcal{S}(h) \quad \text{in } Q(T) := (0,T)\times\Omega, \tag{4.1}$$

where Ω is a bounded domain in $\mathbf{R}^N$ with $N \geq 1$ and f is a given function on $Q(T)$. To obtain (4.1) from (2.3) we assume that ϕ and $\mathcal{H}$ are given positive constants, S in the left hand side is proportional to h and put $g(h) = \frac{\hat{K}_l(h)\phi^2}{\mathcal{H}} + \hat{K}_V C_l \phi(1-S)$. In [15, 14] the graph of $\mathcal{S}$ is illustrated like Figure 2.

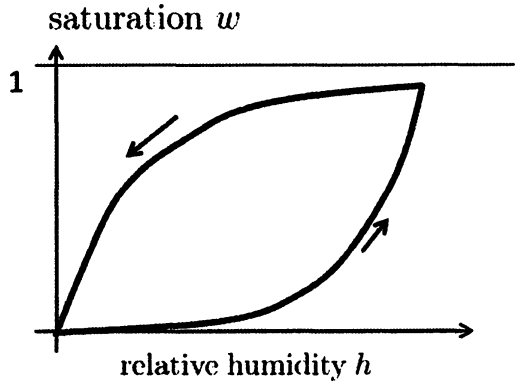

Figure 2: the graph of $\mathcal{S}$

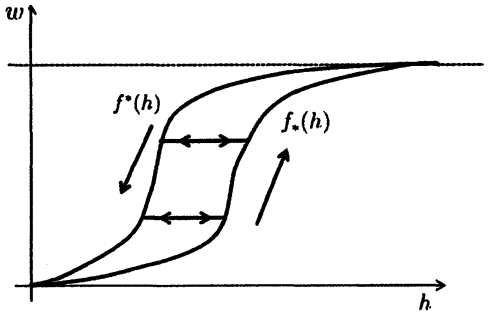

Figure 3: Play operator

From this graph we can observe that the trend of the hysteresis loop is anticlockwise. It is well-known that the hysteresis operator with anticlockwise can be represented by a play operator (see [11, 18], Figure 3). As mentioned in [18, 12, 3], the play operator $w = \mathcal{S}(h)$ is characterized by the ordinary differential equation including a subdifferential of the indicator function. In this paper in order to get the compactness we use the following approximation as the characterization for $\mathcal{S}$.

$$w_t - \nu\Delta w + \partial I(h;w) \ni 0 \quad \text{in } Q(T),$$

where $w_t = (\partial/\partial t)w$, ν is a non-negative constant and $I(h;\cdot)$ is the indicator function of the interval $[f_*(h), f^*(h)]$, f_* and f^* are lower and upper curves indicated in Figure 3, respectively. Moreover, $\partial I(h;\cdot)$ is its subdifferential, that is, it is a multivalued operator given by

$$\partial I(h;r) = \begin{cases} [0,\infty) & \text{for } r = f^*(h), \\ \{0\} & \text{for } f_*(h) < r < f^*(h), \\ (-\infty,0] & \text{for } r = f_*(h). \end{cases}$$

Hence, under consideration of the initial and the boundary conditions we have the following initial boundary value problem PM:

$$\begin{aligned} &\rho h_t - \operatorname{div}(\nabla G(h)) = wf \quad \text{in } Q(T), \\ &w_t - \nu\Delta w + \partial I(h;w) \ni 0 \quad \text{in } Q(T), \\ &h = h_b, w = w_b \quad \text{on } \Sigma(T) := (0,T)\times\partial\Omega, \\ &h(0) = h_0, w(0) = w_0 \quad \text{on } \Omega, \end{aligned}$$

where $G(r) = \int_1^r g(s)ds$ for $r > 0$, h_b and w_b are given functions on $\Sigma(T)$ and h_0 and w_0 are initial functions.

On this problem PM we have proved the following theorems:

Theorem 4.1. *(cf. [1, 2]) Assume:*

(A1) $\Omega \subset \mathbf{R}^N$ *is a bounded domain with the smooth boundary* $\partial\Omega$ *for any positive integer* N.

(A2) ρ *and* ν *are positive constants and* $T > 0$.

(A3) $G : (0,\infty) \to \mathbf{R}$ *is continuous,* $g(r) := G'(r)$ *is continuous on* $(0,\infty)$, $g \in C^2((0,\infty))$ *and* $g(r) \geq g_0$ *for* $r > 0$, *where* g_0 *is a positive constant.*

(A4) $f \in L^\infty(Q(T))$ *with* $f \geq 0$ *a.e. on* $Q(T)$.

(A5) $f_*, f^* \in C^2(\mathbf{R}) \cap W^{2,\infty}(\mathbf{R})$ *with* $0 \leq f_* \leq f^* \leq w_*$ *on* $\mathbf{R}$, *where* w_* *is a positive constant. We put* $L_* = \max\{|f_*|_{W^{2,\infty}(\mathbf{R})}, |f^*|_{W^{2,\infty}(\mathbf{R})}\}$.

(A6) $h_b, w_b \in H^1(\Omega) \cap L^\infty(\Omega)$, $u_b \geq \kappa_0$ *and* $w_b \geq 0$ *a.e. on* Ω, *and* $h_0, w_0 \in H^1(\Omega) \cap L^\infty(\Omega)$, $h_0 \geq \kappa_0$ *and* $w_0 \geq 0$ *a.e. on* Ω *with* $h_0 = h_b$ *and* $w_0 = w_b$ *a.e. on* $\partial\Omega$, *where* κ_0 *is a positive constant. Moreover,* $f_*(h_0) \leq w_0 \leq f^*(h_0)$ *a.e. on* Ω *and* $f_*(h_b) \leq w_b \leq f^*(h_b)$ *a.e. on* $\partial\Omega$. *Then PM has at least one solution on* $[0,T]$.

Theorem 4.2. *(cf. [1, 2]) Let* Ω *be the interval* $(0,1)$ *and assume (A2)* $\sim$ *(A6). If* $\{h_1, w_1\}$ *and* $\{h_2, w_2\}$ *are solutions of PM on [0,T] and* h_1 *and* h_2 *are strictly positive on* $\overline{Q(T)}$, *then it holds that* $h_1 = h_2$ *and* $w_1 = w_2$ *on* $Q(T)$.

As you see Theorem 4.2, the uniqueness holds only in the one-dimensional domain. The next result deals with PM in case $\nu = 0$.

Theorem 4.3. *(cf. [2]) Assume that (A2)* $\sim$ *(A6) hold. Then PM has at least one solution on* $[0,T]$ *even if* $\nu = 0$.

Next, we give a result concerned with (3.1), in which we assume that $\rho_0 = K_g = K_d = 1$, ϕ in the flux term is a constant ($:= 1$). Then we have the following initial-boundary value problem PC:

$$\frac{\partial}{\partial t}\left(\phi(1 - \exp(-\kappa_* \int_0^t u(\tau)d\tau)u\right) - \Delta u = -\kappa_1 w_0 \exp(-\kappa_* \int_0^t u(\tau)d\tau) \quad \text{in } Q(T),$$
$$u = u_b \quad \text{on } \Sigma(T),$$
$$u(0) = u_0 \quad \text{in } \Omega,$$

where u_b and u_0 are given boundary and initial functions with $N = 3$.

On this problem PC the following theorem guarantees the well-posedness.

Theorem 4.4. *(cf. [13]) If* $u_b \in W^{1,2}(0,T; H^1(\Omega)) \cap L^\infty(0,T; H^2(\Omega))$ *with* $0 \leq u_b \leq u_*$ *in* $Q(T)$, *where* u_* *is a positive constant,* $u_0 \in H^1(\Omega) \cap H^2(\Omega)$ *with* $u_0 \geq 0$ *and* $u_0 = u_b(0)$ *on* $\partial\Omega$, *and* $w_0 \in L^\infty(\Omega)$ *is non-negative on* Ω, *then PC has a unique solution on* $[0,T]$.

At the end of this paper we note that a lot of open problems still remain on this topic.

References

[1] T. Aiki, K. Kumazaki, Mathematical model for hysteresis phenomenon in moisture transport of concrete carbonation process, to appear in Physica B.

[2] T. Aiki, K. Kumazaki, Well-posedness of a mathematical model for moisture transport appearing in concrete carbonation process, to appear in Adv. Math. Sci. Appl.

[3] T. Aiki, Mathematical models including a hysteresis operator, Dissipative phase transitions, 1–20, Ser. Adv. Math. Appl. Sci., 71, World Sci. Publ., Hackensack, NJ, 2006.

[4] T. Aiki, A. Muntean, Existence and uniqueness of solutions to a mathematical model predicting service life of concrete structures, Adv. Math. Sci. Appl., 19(2009), 109–129.

[5] T. Aiki, A. Muntean, Large time behavior of solutions to concrete carbonation problem, Communications on Pure and Applied Analysis, Vol. 9, (2010)1117-1129.

[6] T. Aiki, A. Muntean, Mathematical treatment of concrete carbonation process, Current Advances in Nonlinear Analysis and Related Topics, Gakuto International Series, Mathematical Sciences and Applications, Vol. 32, 2010, 231-238.

[7] T. Aiki, A. Muntean, On uniqueness of a weak solution of one-dimensional concrete carbonation problem, Discrete Contin. Dynam. Systems Ser. A, Vol.29, (2010)1345-1365.

[8] T. Aiki, A. Muntean, Mathematical treatment of concrete carbonation process, Current Advances in Nonlinear Analysis and Related Topics, Gakuto International Series, Mathematical Sciences and Applications, Vol. 32, 2010, 231-238.

[9] T. Aiki, A. Muntean, Large time behavior of solutions to concrete carbonation problem, Communications on Pure and Applied Analysis, Vol. 9, (2010)1117-1129.

[10] T. Aiki, A. Muntean, A free-boundary problem for concrete carbonation: Rigorous justification of $\sqrt{t}$-law of propagation, submitted.

[11] M. Brokate and J. Sprekels, *Hysteresis and Phase Transitions*, Springer, Appl. Math. Sci., 121, 1996.

[12] N. Kenmochi, T. Koyama and G. H. Meyer, Parabolic PDEs with hysteresis and quasivariational inequalities, Nonlinear Anal. TMA, 34(1998), 665-686.

[13] K. Kumazaki, On the existence of a solution for a mathematical model of carbon dioxide transport in concrete carbonation process, preprint.

[14] K. Maekawa, R. Chaube, T. Kishi, *Modeling of concrete performance*, Taylor and Francis, 1999.

[15] K. Maekawa, T. Ishida, T. Kishi, Multi-scale modeling of concrete performance, Journal of Advanced Concrete Technology, 1(2003), 91-126.

[16] A. Muntean, A moving-boundary problem: Modeling, analysis and simulation of concrete carbonation, Cuvillier Verlag, Götingen, 2006. PhD thesis, Faculty of Mathematics, University of Bremen, Germany.

[17] A. Muntean, M. Böhm, A moving-boundary problem for concrete carbonation: global existence and uniqueness of solutions, Journal of Mathematical Analysis and Applications, 350(1)(2009), 234-251.

[18] A. Visintin, *Differential Models of Hysteresis*, Appl. Math. Sci., Vol. 111, Springer-Verlag, Berlin, 1993.